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Evaluation of the 2018 Version of the Integrated Surveillance Program Database Pressure Equation

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1.0 Introduction

The Integrated Surveillance Program (ISP) Database Pressure Equation was developed to determine with reasonable certainty the total maximum pressure of hydrogen and other gases in packaged 3013 containers stored at Savannah River Site (SRS) in support of the destructive evaluation (DE) process. The pressure equation in the Department of Energy (DOE) 3013 Standard, "Standard for Stabilization, Packaging and Storage of Plutonium-Bearing Materials" (DOE-STD-3013-2004) used a bounding assumption that all the water is decomposed to form hydrogen.[1] However, the results of Los Alamos National Laboratory (LANL) shelf-life experiments showed that hydrogen is consumed, and that the maximum pressures would not approach the design pressure of the 3013 container.[2] Therefore, the ISP Database Pressure Equation was revised in 2008 to include terms for the generation of helium and hydrogen as a function of time, as well as the consumption of water and destruction of hydrogen based on shelf-life results. The 2008 ISP Database Pressure Equation provided a more reasonable estimate of the total maximum pressure in packaged 3013 containers than the pressure equation in versions of the 3013 Standard issued prior to 2018.

In 2018, the current 3013 Standard (DOE-STD-3013-2018) was published with a revised pressure equation.[3] The revised equation includes two empirical factors that reduce the calculated formation of hydrogen and release of helium to the gas phase. The empirical factor η_{H_2} reduces the formation of hydrogen as a function of total moisture, based on results of 3013 destructive evaluations and LANL shelf-life experiments. The factor η_{He} reduces the helium release based on observations of helium in sealed ^{238}Pu oxide fuel containers.[4] The Surveillance Program Authority has requested that the pressure equation from DOE-STD-3013-2018 be implemented in the ISP database. The database code has been updated to incorporate the new methodology. This document evaluates the database code through a hand calculation and provides a comparison of calculated pressures and measured pressures for containers that have undergone destructive evaluation.

1.1 Purpose

This calculation documents the methodology and computer code for the 2018 Version of the ISP Database Pressure Equation, which is used to determine the maximum pressure of hydrogen and other gases packaged in 3013 containers in storage at SRS. The 2018 Version of the ISP Database Pressure Equation uses the methodology as written in DOE-STD-3013-2018.[3] The formula for the calculation of the average gas temperature from the previous pressure equation described by Friday[2] is retained. The equations in DOE-STD-3013-2018 are specifically for calculating the pressure in the outer container, but the maximum pressures within the inner container are also of interest. The inner container pressures are obtained using a free gas volume specific to the inner container, which is calculated using the same approach outlined in DOE-STD-3013-2018 for the outer container. This document also provides total maximum pressures of all 3013 containers that have undergone DE to date and compares those pressures to those measured in DE.

2.0   Methodology

2.1   Total Maximum Pressure in the 3013 Inner Container

The methodology for calculating the total maximum pressure is described in detail in
DOE-STD-3013-2018.[3] The pressure equation is the sum of three terms A, B and C,
shown below in Eq. (1)

$$P_{IC} = P_F + \eta_{H_2} P_{H_2} + \eta_{He} P_{He}$$

$$\phantom{P_{IC} = P_F}\text{(A)}\quad\text{(B)}\qquad\text{(C)}$$

(1)

where

   P_{IC} is the total maximum pressure in the inner container (absolute),
   P_F is the partial pressure of the fill gas [kPa],
   P_{H_2} is the partial pressure of the generated hydrogen gases [kPa],
   P_{He} is the partial pressure of helium produced by alpha decay [kPa],
   η_{H_2} is the fraction of water that decomposes to form hydrogen gas (determined
   empirically), and
   η_{He} is the fraction of helium from alpha decay that enters the gas phase
   (determined empirically).

The 3013 Standard derives an aggregate equation based on Eq. (1) in terms of measured
and calculated quantities in the ISP Database for the specific 3013 container geometry
and properties of the packaged materials. The aggregate equation with terms A, B, and C
expanded is shown below in Eq. (2)

$$P_{IC} = P_0 \frac{T_1}{T_0} + \eta_{H_2} \frac{m \cdot w_{H_2O}}{M_{H_2O}} \cdot \frac{RT_1}{V_g} + \eta_{He} \cdot 6.232 \times 10^{-5} \left[\frac{\text{mol}}{\text{yr} \cdot \text{W}} \right] \cdot \frac{QtRT_1}{V_g}$$

$$\text{(A)}\quad |\text{--------(B)--------}| \quad |\text{----------------(C)------------------}|$$

(2)

where
   P_0 is the initial pressure at the time the container is sealed [kPa],
   T_0 is the initial average temperature of the gas within the container at the time the
   container is sealed [K],
   T_1 is the average temperature of the gas within the container at the time the
   container is evaluated [K],
   m is the net weight of the material [g],
   w_x is the mass fraction of component x,
   M_x is the atomic or molecular weight of component x [g mol^{-1}],
   R is the universal gas constant, 8.3145 [kPa L K^{-1} mol^{-1}],
   V_g is the free gas volume of the container [L],
   Q is the total material thermal power [W], and
   t is the time since container was sealed [y].

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The average temperature of the gas within the container at the time the container is evaluated is determined as a function of the total material thermal power as shown in Eq. (3).[2]

$$T_1 = 3Q + 1.6Q + 25 + 273 \tag{3}$$

The symbol V_g represents the free gas volume of the container. The free gas volumes are the minimum unoccupied volumes of the inner and outer containers. These values are container and site specific and handled by the ISP database as input values for each container. The ISP Database uses these values to calculate the total maximum pressure separately for both the inner and outer 3013 containers. Calculations of the minimum unoccupied volumes of the 3013 outer container and 3013 inner container are shown in Table 3 and Table 4, respectively.

The volume of the contained material V_m is calculated by m/ρ, where ρ is the particle density of the material.

The particle density of the material is estimated based on the material composition and the crystal density of each component as shown in Eq. (4) below.

$$\rho = \cfrac{1}{\cfrac{w_{PuO_2}}{\rho_{PuO_2}} + \cfrac{w_{U_3O_8}}{\rho_{U_3O_8}} + \cfrac{w_{NpO_2}}{\rho_{NpO_2}} + \cfrac{w_{AmO_2}}{\rho_{AmO_2}} + \cfrac{w_{H_2O}}{\rho_{H_2O}} + \cfrac{w_{salt}}{\rho_{salt}}} \tag{4}$$

Equation 4 can be used to calculate the density of packaged material when the sum of the mass fractions of the constituents is less than 1.0. This is referred to as condition 1. However, evaluation of the data in the ISP database has shown that the sum of the mass fractions of the constituents frequently exceeds 1.0. Reasons for this discrepancy may include (a) random error in the assays or (b) the uncertainty in the uranium assay.[2] Uncertainty in the uranium assay often exceeds those of the other actinides because of the use of a nondestructive assay method rather than analytical chemistry for the materials packaged in 3013 containers.

Therefore, corrections to the particle density are made when w_{T-S}, the mass fraction of the total minus the salt (or the fraction of all of the actinide oxides plus water) exceeds 1.00. In the case for random error in the assays (Case a), w_{T-S} would be expected to exceed 1.00 by only a small amount (i.e. < 0.02). Therefore, the error in the total mass balance ($w_{T-S} - 1$) is less than 0.02. The salt term is removed, and the weight fractions of each of the components are adjusted by w_{T-S} proportionally as shown in Eq. (4)$_a$. This is referred to as condition 2.

$$\rho = \cfrac{1}{\cfrac{w_{PuO_2}/w_{T-S}}{\rho_{PuO_2}} + \cfrac{w_{U_3O_8}/w_{T-S}}{\rho_{U_3O_8}} + \cfrac{w_{NpO_2}/w_{T-S}}{\rho_{NpO_2}} + \cfrac{w_{AmO_2}/w_{T-S}}{\rho_{AmO_2}} + \cfrac{w_{H_2O}/w_{T-S}}{\rho_{H_2O}}} \tag{4$_a$.}$$

When the discrepancy is due to errors in the uranium assay (Case b), the error in the total mass balance ($w_{T-S} - 1$) is larger than what would be expected due to random error. The

error in the total mass balance $(w_{T-S} - 1)$ is greater than 0.02, but it is less than uranium assay $w_{U_3O_8}$. Therefore, the salt term is removed, and the uranium term is adjusted by $(w_{T-S} - 1)$ as shown in Eq. (4)$_b$. This is referred to as condition 3.

$$\rho = \cfrac{1}{\cfrac{w_{PuO_2}}{\rho_{PuO_2}} + \cfrac{w_{U_3O_8} - (w_{T-S} - 1)}{\rho_{U_3O_8}} + \cfrac{w_{NpO_2}}{\rho_{NpO_2}} + \cfrac{w_{AmO_2}}{\rho_{AmO_2}} + \cfrac{w_{H_2O}}{\rho_{H_2O}}} \qquad (4)_b.$$

In some cases, the discrepancy $(w_{T-S} - 1)$ is greater than 0.02, but it cannot be explained by errors in the uranium assay. This occurs because the discrepancy $(w_{T-S} - 1)$ exceeds the uranium assay, $w_{U_3O_8}$. In this case, the salt term is removed, and the weight fractions of each of the components is adjusted by w_{T-S}, proportionally as shown in (4)$_a$ This is referred to as condition 4.

The particle density calculated from Eqs. (4), (4)$_a$, and (4)$_b$ is referred to in the database as the "best density". These values are reduced by 10% per DOE-STD-3013-2018 to obtain a more conservative particle density, which is simply referred to as the "density".

2.2 Total Maximum Pressure in the 3013 Outer Container for a Failed 3013 Inner Container

If an inner 3013 container has or develops a leak, the gases in the inner container will escape into the annular region between the outer container and the inner container. Assuming a sufficiently large leak in the inner container occurs, the pressure P_{IC} in the inner container will come to equilibrium with that of the annular region P_{OI}. The resulting pressure inside the outer container P_{OC} is calculated from the sum of the moles of gas originally inside the inner container n_{IC} and the moles of gas originally in the annular region n_{OI} based on the ideal gas law as shown in Eq. (5).

$$P_{OC} = (n_{OI} + n_{IC}) \frac{RT_1}{V_{U,OC}} \qquad (5)$$

The moles of gas originating inside the inner container n_{IC} can be determined from the inner container pressure P_{IC} using the ideal gas law as follows.

$$n_{IC} = \frac{P_{IC} V_{U,IC}}{RT_1} \qquad (6)$$

Likewise, the moles of gas originating inside the annular region n_{OI} can be calculated using the ideal gas law by substituting the original pressure of the outer container P_{OC} and the volume of the annular region V_{OI}. The original pressure of the outer container P_{OC} is the local atmospheric pressure at the site of packaging. The original pressure P_{OC} can be adjusted for the heating of the container using the ideal gas law. The volume of the annular region V_{OI} is the difference of the minimum unoccupied volume of the 3013 outer container $V_{U,OC}$ and the minimum unoccupied volume of the 3013 inner container $V_{U,IC}$. Substituting these values gives an expression for calculating n_{OI} as shown in Eq. (7).

$$n_{OI} = \frac{P_{OI}V_{OI}}{RT} = \frac{P_0 V_{OI}}{RT_0} = \frac{(T_0/T_1)P_F V_{OI}}{RT_0} = \frac{P_F(V_{U,OC} - V_{U,IC})}{RT_1} \tag{7}$$

Substituting Eqs. (6) and (7) into Eq. (5) gives the resulting pressure inside the outer container.

$$P_{OC} = \frac{P_F(V_{U,OC} - V_{U,IC}) + P_{IC}V_{U,IC}}{V_{U,OC}} \tag{8}$$

3.0   Acceptance Criteria

There are no acceptance criteria associated with this calculation.

4.0   Unverified Assumptions

There are no unverified assumptions associated with this calculation.

5.0   Assumptions

The following assumptions apply to the ISP Database Pressure Equation based on DOE-STD-3013-2018.[3]

  I.   The gases within the sealed 3013 containers follow the ideal gas law.

 II.   The three gas sources requiring consideration in this calculation include (1) the container fill gas, (2) any gases evolved during storage, and (3) helium produced by alpha decay of the radioactive species within the packaged 3013 containers.

III.   The only evolved gas of significance during extended storage is hydrogen, which is produced through the radiolysis of adsorbed water.

 IV.   Any oxygen produced through the radiolysis of water is consumed by the material.

  V.   Actinide oxides have the following chemical forms: plutonium oxide, PuO_2; uranium oxide, U_3O_8; americium oxide, AmO_2; and neptunium oxide, NpO_2.

6.0   Limitations

This calculation applies to sealed containers of pure and impure plutonium oxide packaged inside 3013 containers per the requirements of DOE-STD-3013-2018.[3] This calculation applies to 3013 container configurations listed in Table B-2 of DOE-STD-3013-2018 with their associated volumes.

7.0   Calculation Inputs

7.1   Constants

The following calculation inputs are constants used in the ISP Database Pressure Equation are listed in Table 1.

Table 1. ISP Database Pressure Equation Constants.

Symbol	Quantity	Description
T_0	298 K	Initial average temperature of the gas within the container at the time the container is sealed
M_{H_2O}	18.0152 g mol^{-1}	Molecular weight of water
R	8.3145 kPa L K^{-1} mol^{-1}	Universal gas constant
ρ_{PuO_2}	11.5 g cm^{-3}	Particle density of plutonium oxide
$\rho_{U_3O_8}$	8.38 g cm^{-3}	Particle density of uranium oxide
ρ_{AmO_2}	11.7 g cm^{-3}	Particle density of americium oxide
ρ_{NpO_2}	11.1 g cm^{-3}	Particle density of neptunium oxide
ρ_{SS}	8.0 g cm^{-3}	Density of stainless steel
ρ_{H_2O}	1.0 g cm^{-3}	Density of water
ρ_{Salt}	2.5 g cm^{-3}	Density of salt components (average)
η_{He}	0.5	fraction of helium from alpha decay that enters the gas phase (determined empirically)
$(O/M)_{PuO_2}$	1.134	Oxygen to metal weight ratio for plutonium oxide
$(O/M)_{U_3O_8}$	1.179	Oxygen to metal weight ratio for uranium oxide
$(O/M)_{AmO_2}$	1.132	Oxygen to metal weight ratio for americium oxide
$(O/M)_{NpO_2}$	1.135	Oxygen to metal weight ratio for neptunium oxide

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7.2   Input Variables

The following calculation inputs are variables used in the ISP Database Pressure Equation obtained directly from tables in the ISP Database.

Table 2. ISP Database Pressure Equation Input Variables

Symbol	ISP Database Field	Description
P_0	AtmosPress_kPa_@298K:	Local atmospheric pressure at the site of packaging
	IIf([tblPCDProcessed].[SiteID]=1 Or [tblPCDProcessed].[SiteID]=3, 99,	Hanford Plutonium Finishing Plant or Lawrence Livermore National Laboratory (LLNL) 99 kPa
	IIf([tblPCDProcessed].[SiteID]=2, 78,	Los Alamos National Laboratory (LANL) (PF4) 78 kPa
	IIf([tblPCDProcessed].[SiteID]=4, 81,	Rocky Flats (RFETS) Plant 81 kPa
	IIf([tblPCDProcessed].[SiteID]=5, 101,	Savannah River Site (SRS) (FB-Line) 101 kPa
	-9999))))	error condition
Q	[tblPCDCalGamma]! [Wattage]	Total material thermal power [W]
t_{eval}	[Pressure Calculation End Date] *(User input)*	Date (and time) at which pressure in container is evaluated
t_{weld}	[tblPCDInnerCan]! [InnerCanDateTimeofweld]	Date and time the inner weld was completed
m	[tblPCDConvCan]! [ConvCanNet]	Net weight [g] of the material in the convenience can
m_{Pu}	[tblPCDCalGamma]! [Pu Measured (g)]	Total measured weight [g] of plutonium
m_U	[tblPCDCalGamma]! [U Measured (g)]	Total measured weight [g] of uranium
m_{Am}	[tblPCDCalGamma]! [Am Measured (g)]	Total measured weight [g] of americium
m_{Np}	[tblPCDCalGamma]! [Np Measured (g)]	Total measured weight [g] of neptunium
$wt\%_{H_2O}$	[tblPCDMoisture]! [MoisturePercent]	Percent moisture in 3013 container
$V_{U,IC}$	[tblPCDProcessed]! [VolInnerCont]	Minimum unoccupied volume [L] inside a 3013 inner container with a nested convenience container (container and site specific). See Table 4.
$V_{U,OC}$	[tblPCDProcessed]! [VolInnerCont]	Minimum unoccupied volume [L] inside a 3013 outer with nested inner and convenience containers (container and site specific)

It is noted that SRS did not report the masses of americium and neptunium for all items. These values are used in the density calculation, Eqs. (4), (4)$_a$, and (4)$_b$. A review of the existing data shows that the americium accounts for up to 10% of the material and the neptunium accounts for up to 3% of the material in any given 3013 container. For containers with principally PuO$_2$, the impact on the density calculation and the inner

container pressure of unreported AmO_2 is very small due to the small difference in the density between PuO_2 and AmO_2. For containers with a large fraction of salt, unreported americium is assumed to be salt. This results in calculated densities being smaller and calculated pressures being higher than if the americium had been reported. Thus, the reported values for the calculated pressures for the sites that did not report americium are bounding. Although the amount of pressure increase can be significant for a 3013 loaded with 5 kg of material with 30 wt% salt, there are no containers with these characteristics in the existing 3013 inventory.

Table 3. Calculation of the Minimum Unoccupied Volume of the 3013 Outer Container: $V_{U,OC} = V_{OC} - U_0 - V_i - U_1 - V_{cc} - U_2.$[3]

Component		RFETS	Hanford	SRS	LLNL	LANL	ARIES
Outer Container Interior Volume	V_{OC}	2.608	2.608	2.608	2.608	2.608	2.608
Uncertainty (due to container fabrication tolerances)	U_0	0.012	0.012	0.012	0.012	0.012	0.012
Inner Container Material Volume	V_i	0.143	0.216	0.216	0.143	0.11	0.11
Uncertainty (due to container fabrication tolerances)	U_1	0.045	0.015	0.015	0.045	0.031	0.031
Convenience Container Material Volume	V_{cc}	0.218	0.191	0.106	0.218	0.022	0.067
Uncertainty (due to container fabrication tolerances)	U_2	0.022	0.019	0.011	0.022	0.002	0.007
Minimum Unoccupied Volume of the 3013 Outer Container	$V_{U,OC}$	**2.168**	**2.155**	**2.248**	**2.168**	**2.432**	**2.382**

Note: DOE-STD-3013-2018 uses the symbol V_C to represent the Minimum Unoccupied Volume of the 3013 Outer Container.

Table 4. Calculation of the Minimum Unoccupied Volume of the 3013 Inner Container: $V_{U,IC} = V_{IC} - V_{cc} - U_2.$

Component		RFETS	Hanford	SRS	LLNL	LANL	ARIES
Inner Container Interior Volume	V_{IC}	2.174	2.089	2.086	2.174	2.242	2.242
Convenience Container Material Volume	V_{cc}	0.218	0.191	0.106	0.218	0.022	0.067
Uncertainty (due to container fabrication tolerances)	U_2	0.022	0.019	0.011	0.022	0.002	0.007
Minimum Unoccupied Volume of the 3013 Inner Container	$V_{U,IC}$	**1.934**	**1.879**	**1.972**	**1.934**	**2.218**	**2.168**

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7.3 Calculated Inputs

The following are calculated input variables used in the ISP Database Pressure Equation.

Table 5. ISP Database Pressure Equation Calculated Input Variables

Symbol	Description	Calculation	ISP Database Calculation
η_{H_2}	Fraction of water that decomposes to form hydrogen gas (determined empirically)	$(0 < w_{H_2O} \leq 0.31)$: 0.13 $(w_{H_2O} > 0.31)$: $0.60 \cdot 100 \cdot w_{H_2O} - 0.056$	**n-H2:** IIf([tblPCDMoisture]![MoisturePercent]<0, 0, IIf([tblPCDMoisture]![MoisturePercent]<0.31, 0.13, 0.6*[tblPCDMoisture]![MoisturePercent]-0.056))
t	Elapsed time from date of inner can welding to date of evaluation [d]	$t_{eval} - t_{weld}$	**date dif:** DateDiff("d",[tblPCDInnerCan]![InnerCanDateTimeofweld], [Pressure Calculation End Date])/365.25
T_1	Average temperature of the gas within the container at the time the container is evaluated [K]	See Eq(3).	**T:** [tblPCDCalGamma]![Wattage]*3+[tblPCDCalGamma]![Wattage]*1.6+25+273
V_g	Free gas volume of the container [L]	$V_{U,IC} - m/\rho$	**V-GasI:** [tblPCDProcessed]![VolInnerCont]-[tblPCDConvCan]![ConvCanNet]/([Density]*1000)
w_{Pu}	Mass fraction of plutonium	m_{Pu}/m	**f-Pu:** Nz([Pu Measured (g)])/Nz([ConvCanNet])
w_U	Mass fraction of uranium	m_U/m	**f-U:** Nz([U Measured (g)])/Nz([ConvCanNet])
w_{Am}	Mass fraction of americium	m_{Am}/m	**f-Am:** Nz([Am Measured (g)])/Nz([ConvCanNet])
w_{Np}	Mass fraction of neptunium	m_{Np}/m	**f-Np:** Nz([Np Measured (g)])/Nz([ConvCanNet])
w_{PuO_2}	Mass fraction of plutonium oxide	$m_{Pu}/m \cdot (O/M)_{PuO_2}$	**f-PuO2:** Nz([Pu Measured (g)])/Nz([ConvCanNet])*1.134
$w_{U_3O_8}$	Mass fraction of uranium oxide	$m_U/m \cdot (O/M)_{U_3O_8}$	**f-U3O8:** Nz([U Measured (g)])/Nz([ConvCanNet])*1.179
w_{AmO_2}	Mass fraction of americium oxide	$m_{Am}/m \cdot (O/M)_{AmO_2}$	**f-AmO2:** Nz([Am Measured (g)])/Nz([ConvCanNet])*1.132
w_{NpO_2}	Mass fraction of neptunium oxide	$m_{Np}/m \cdot (O/M)_{NpO_2}$	**f-NpO2:** Nz([Np Measured (g)])/Nz([ConvCanNet])*1.135

Symbol	Description	Calculation	ISP Database Calculation
w_{H_2O}	Mass fraction of water	$(wt\%_{H_2O})/100$	**f-H2O:** IIf([tblPCDMoisture]![MoisturePercent]<0,0,[tblPCDMoisture]![MoisturePercent]/100)
w_{ActOx}	Mass fraction of actinide oxide; Sum of the plutonium oxide, uranium oxide, americium oxide and neptunium oxide mass fractions.	$w_{PuO_2} + w_{U_3O_8} + w_{AmO_2} + w_{NpO_2}$	**f-ActOx:** (Nz([Pu Measured (g)])/Nz([ConvCanNet]))*1.134+ (Nz([U Measured (g)])/Nz([ConvCanNet]))*1.179+ (Nz([Am Measured (g)])/Nz([ConvCanNet]))*1.132+ (Nz([Np Measured (g)])/Nz([ConvCanNet]))*1.135
w_{T-S}	The mass fraction of the total minus the salt; The fraction of all of the actinide oxides plus water)	$w_{ActOx} + w_{H_2O}$	**f-T-S:** [f-ActOx]+[f-H2O]
w_S	The mass fraction of the salt	$1 - w_{T-S}$	**f-Salt:** IIf([f-T-S]<1,1-[f-T-S],0)

7.4   Density

<u>Best Density</u>: See Equations (4), (4)$_a$, and (4)$_b$.

Best_Density:
IIf([f-T-S]<1,
          1/(([f-PuO2]/11.5)+([f-U3O8]/8.38)+([f-AmO2]/11.7)+([f-NpO2]/11.1)+((1-[f-T-S])/2.5)+[f-
          H2O]),
          IIf([f-T-S]-1<0.02,
                    1/((([f-PuO2]/[f-T-S])/11.5)+(([f-U3O8]/[f-T-S])/8.38)+(([f-AmO2]/[f-T-S])/11.7)+(([f-
                    NpO2]/[f-T-S])/11.1)+([f-H2O]/[f-T-S])),
                    IIf([f-U3O8]<[f-T-S]-1,
                              1/((([f-PuO2]/[f-T-S])/11.5)+(([f-U3O8]/[f-T-S])/8.38)+(([f-AmO2]/[f-T-
                              S])/11.7)+(([f-NpO2]/[f-T-S])/11.1)+([f-H2O]/[f-T-S])),
                              1/(([f-PuO2]/11.5)+(([f-U3O8]-([f-T-S]-1))/8.38)+([f-AmO2]/11.7)+([f-
                              NpO2]/11.1)+[f-H2O])))))

<u>Density</u>: The best density is multiplied by a factor of 0.9 to give the density of the material.

Density:

[Best_Density]*0.9

8.0   Computer Hardware and Software

The ISP Database Pressure Equation query is written in structured query language (SQL) and runs in IA Standard Microsoft Office Access 2007-2016 running on a Windows PC.

9.0   Calculation

The ISP Database Pressure Equation query calculates the inner container pressure for each 3013 container packaged with nonmetal contents using the calculation inputs defined in Section 7. The aggregate equation for the inner container pressure P_{IC} based on Eq. (2) is coded in the ISP Database Pressure Equation query as follows:

A: [AtmosPress_kPa_@298K]*[T]/298

B: [n-H2]*([ConvCanNet]*[f-H2O]/18.0152)*8.314*[T]/[V-GasI]

C: 0.5*0.00006232*[Wattage]*[date dif]*8.314*[T]/[V-GasI]

TAP_IC_kPa: [A]+[B]+[C]

The resulting ISP Database Pressure Equation query also calculates the resulting pressure of the outer 3013 container assuming that a gross leak had developed in the inner container based on Eq. (8). This equation is coded in the ISP Database Pressure Equation query as follows:

TAP_OC_kPa:
([A]*([VolOuterCont]-[VolInnerCont])+[TAP_IC_kPa]*[VolInnerCont])/[VolOuterCont]

A hand calculation was performed comparing the results of the ISP Database Pressure Equation evaluated for each of the four conditions for the density equation. The results of the hand calculation are given in Appendix 1. For each example given, the Table on the left is the output from the query and the Table on the right is the hand calculation.

10.0 Summary and Conclusions

A SQL query that returns the calculated pressure in the outer container and the inner container at a specified time has been described. The query has been run for all of the containers (3,772) in the ISP Database using an end date of January 1, 2021. The pressures are plotted from the lowest calculated pressure to the highest calculated pressure in Figure 1. No inner container pressure approaches the 790 kPa (100 psig) internal pressure that is required to be detectable by non-destructive means.[5] Over 99% of the containers (3,752 out of 3,772) in the ISP Database have calculated inner container pressures less than 250 kPa, which is less than one third of the 790 kPa requirement. The highest calculated pressure of 431 kPa belongs to H003328, the Hanford High Moisture Container originally packaged with 0.52 wt% moisture. This container has undergone DE, and the observed pressure was 299 kPa. The second highest calculated pressure of 332 kPa belongs to R610548, originally packaged with 0.14 wt% moisture. The pressure is a result of the low calculated gas volume within the inner container of 0.58 L, which is mainly due to the high salt fraction of over 50% resulting in a low density. Of the remaining 18 containers with an inner container pressure of greater than 250 kPa, six are from SRS and 12 are from Rocky Flats (RFETS). They range in Best Moisture from 0.20 to 0.32 wt%. However, both SRS and RFETS inner container pressures are consistently measured in DE to be much less than calculated due to the way the Best Moisture measurement was made, which is consistently measured high. Four of these 18 containers have undergone DE and the pressures measured at DE can be compared to the calculated pressures, Table 6. The pressures for these four RFETS and SRS containers are less than atmospheric pressure and typically less than one-third of the calculated pressure. Thus, for the 18 containers from SRS and RFETS with calculated inner container pressures greater than 250 kPa, the calculated pressure is most likely too high.
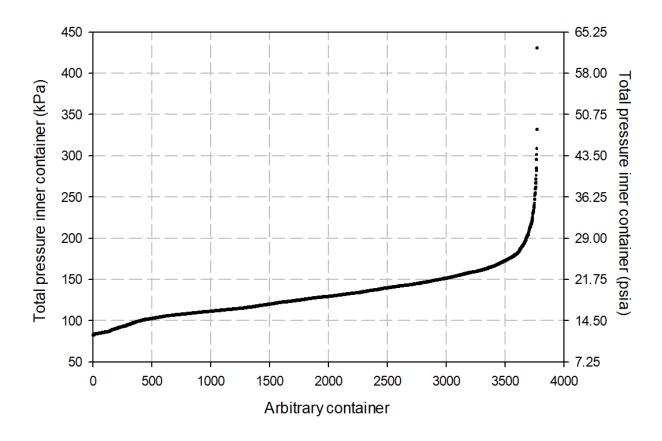
Figure 1. The total pressure within the inner container for all 3,772 containers in the ISP Database plotted from the lowest to the highest calculated pressure.

Table 6. Containers with Calculated Pressures Exceeding 250 kPa That Have Undergone DE Compared to the Pressures Measured at the Time of Destructive Evaluation (DE)

Container ID	FY-DE	Calculated pressure (kPa)	Measured pressure (kPa)
H003328	11-13	431	299
R600793	17-06	332	90
S002129	11-02	296	85
S002277	14-06	282	84
S001105	11-05	267	83

There are two containers where the calculated inner container pressure is slightly lower than the observed inner container pressure at DE, both RFETS containers. The two containers and the pressure differences are FY08DE04 R610327 with a 0.2 kPa difference (Best Moisture 0.003 wt%) and FY10DE06 R610627 with a 0.9 kPa difference (Best Moisture 0.016 wt%). The population of RFETS containers has been shown to have pressures at welding that exceeded the local atmospheric pressure.[5] Thus, it is expected that the assumption of atmospheric pressure at welding could result in low calculated pressures for those containers with low amounts of moisture. The calculated hydrogen

and helium content is not sufficient to make up for the difference between the actual fill gas pressure and the local atmospheric pressure.

The calculated pressure is strongly dependent upon the inner container free gas volume. The free gas volume can be strongly dependent upon the calculated material density and the amount of material in the container. If the calculated material density is low, then the free gas volume can be lower than reasonable. The lowest measured material density during DE is greater than 4 g cm^{-3}. Thus, a calculated material density of less than 4 g cm^{-3}, which may arise due to assumptions made in the calculation, is probably in error. There are 84 containers with a calculated "best density" of less than 4 g cm^{-3}. All 84 containers have a salt fraction that is greater than 51%. There are three containers with a salt fraction greater than 70%, which violates the 3013 requirement to have a minimum of 30 wt% of plutonium plus uranim. Impurities with densities greater than the assumed average salt density of 2.5 g cm^{-3} that are assigned to the salt fraction will result in calculated densities that are too low. The data suggest three materials could be responsible for low calculated densities – uranium oxide (8.4 g cm^{-3}), fluoride salts (35% more dense than the chloride salts for the four most common cations), and magnesium oxide (3.6 g cm^{-3}). Of the 84 containers, 47 are from the Pressure bin which has no chlorine by definition. Of the remaining 37 containers, 16 are in the Pressure and Corrosion bin due to fluorine (no chlorine), and 10 are washed materials from Lawrence Livermore National Laboratory (LLNL), which should have minimal chlorine left due to the high solubility of chloride salts. Four of the five containers with the smallest calculated density are from the PuUOx-HN-Misc represented group, meaning they should contain uranium oxide. Three of these have no reported uranium. Any uranium oxide (density 8.4 g cm^{-3}) missing in the reported actinides is assumed to be salt with a density of 2.5 g cm^{-3}. Twenty-nine of the containers are from the MgOHPPt-HN represented group, which should have a large fraction of MgO after calcination. The MgO material is assumed to be salt.

In contrast, a calculated material density that is too high would result in a higher free gas volume than what is reasonable. This condition occurs when the weight fraction of all of the actinide oxides plus water w_{T-S} is greater than 1, and the material contains salt components. As described earlier, values of w_{T-S} greater than 1 are assumed to be due to the error in the assays of the actinide components; therefore the salt components are removed from the density equation as shown in Eqs. (4)$_a$, and (4)$_b$. However, 17 containers in the pressure and corrosion bin have values of w_{T-S} greater than 1. Eight of these containers have greater than 1 wt% chloride or fluoride salt components as determined by prompt gamma analysis. The three containers with the highest chlorine or fluorine concentrations in this group are given in Table 7. The calculated pressure with the salt component removed is the fourth column. The pressure was recalculated with the salt component included and is given in the fifth column. Neglecting the salt component results in a lower calculated pressure. However, this condition occurs for a small number of items, and correcting for the impurities does not make sufficient difference to change the calculation.

Table 7. Calculated and Corrected Pressures for Salt-Bearing Containers with the Salt Fraction Neglected in the Density Calculation

Container ID	Moisture (wt%)	Cl/F Components	Calculated Pressure (kPa)	Corrected Pressure (kPa)
R610681	0.07	1.5 wt% F	118	121
H000917	0.01	2.9 wt% Cl	86	90
S002220	0.07	9.7 wt% F	134	148

The relationship between the inner container hydrogen pressure and the moisture percentage is complex as shown in Figure 2. There are three general trends in Figure 2 that arise from differences in the amount of material and the amount of impurities. Small amounts of relatively pure material result in the lower calculated hydrogen pressures, for instance at 0.3 wt% moisture a pressure of 30 kPa. A half full container with 30 wt% chlorides gives pressures in the middle range, for instance at 0.3 wt% moisture a pressure of 100 kPa. Full containers with high impurities give the highest pressures, for instance at 0.3 wt% moisture a pressure of 200 kPa. The point at 230 kPa and 0.14 wt% has been discussed, and the high pressure is due to the low gas volume due to low material density. Three factors that contribute to high hydrogen pressures are (1) high moisture content, (2) high mass loading, and (3) low fill gas volumes (high salt content). If all three factors are present, then there is a possibility to exceed the 790 kPa internal pressure that is required to be detectable by non-destructive means. No container currently packaged has all three factors present.
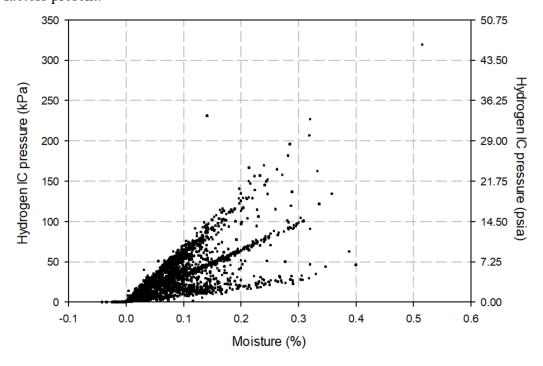

Figure 2. The calculated hydrogen pressure, Term B, versus the moisture percentage for all 3,772 containers in the ISP Database.

11.0 References

1.   *Stabilization, Packaging, and Storage of Plutonium-Bearing Materials*; DOE-STD-3013-2004; U. S. Department of Energy: Washingon, D.C., 2004.
2.   Friday, G. P.; Peppers, L. G.; Veirs, D. K. *A Method for Estimating Gas Pressure in 3013 Containers Using an ISP Database Query*; WSRC-STI-2008-00214; Savannah River National Laboratory: Aiken, SC, July 2008, 2008.
3.   *Stabilization, Packaging, and Storage of Plutonium-Bearing Materials*; DOE-STD-3013-2018; U. S. Department of Energy: Washingon, D.C., 2018.
4.   Mulford, R. N. *Helium Transport in PuO2 as a Function of Temperature and Heating Rate*; LA-UR-14-25325; Los Alamos National Laboratory: Los Alamos, NM, 2014.
5.   Veirs, D. K.; Kelly, E. J.; Berg, J. M.; Nguyen, B.; McClard, J. W.; Hensel, S. J.; Duffey, J. M.; Scogin, J. H. *Gas Composition Observed by Destructive Examination of 3013 Containers*; LA-UR-17-31465; Los Alamos National Laboratory: Los Alamos, NM, 2017.

Appendix 1. Calculation Examples

Calculation Example 1: Density Condition 1

3013ContainerID	TEST04

Date of Evaluation	01-Jan-21	Input variable	Input variable	01-Jan-21	
Date of Evaluation (numeric)	44197.00	Input variable	Input variable	44197.00	
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
InnerCanDateTimeofweld (numeric)	37622.00	Input variable	Input variable	37622.00	
3013ContainerID	TEST04	Input variable	Input variable	TEST04	
SiteID	Hanford	Input variable	Input variable	Hanford	
Wattage	10.00	Input variable	Input variable	10.00	W
Pu Measured (g)	2000.00	Input variable	Input variable	2000.00	g
U Measured (g)	0.00	Input variable	Input variable	0.00	g
Np Measured (g)	0.00	Input variable	Input variable	0.00	g
Am Measured (g)	5.00	Input variable	Input variable	5.00	g
MoisturePercent	0.4000	Input variable	Input variable	0.4000	wt.%
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
ConvCanNet	3000.00	Input variable	Input variable	3000.00	g
T	344.000	$T_1 = 3Q + 1.6Q + 25 + 273$	$T_1 = 3 \cdot 10 + 1.6 \cdot 10 + 25 + 273$	344.000	K
f-H2O	0.00400	$w_{H_2O} = (wt\%_{H_2O})/100$	$w_{H_2O} = (0.4000)/100$	0.00400	
f-Pu	0.667	$w_{Pu} = m_{Pu}/m$	$w_{Pu} = 2000/3000$	0.667	
f-Am	0.00167	$w_{Am} = m_{Am}/m$	$w_{Am} = 5/3000$	0.00167	
f-U	0.00000	$w_U = m_U/m$	$w_U = 0/3000$	0.00000	
f-Np	0.00000	$w_{Np} = m_{Np}/m$	$w_{Np} = 0/3000$	0.00000	

Calculation Example 1: Density Condition 1 continued (2).

f-PuO2	0.756	$w_{PuO_2} = m_{Pu}/m \cdot (O/M)_{PuO_2}$	$w_{PuO_2} = 2000/3000 * 1.134$	0.756
f-AmO2	0.00189	$w_{AmO_2} = m_{Am}/m \cdot (O/M)_{AmO_2}$	$w_{AmO_2} = 5/3000 * 1.132$	0.00189
f-U3O8	0.00000	$w_{U_3O_8} = m_U/m \cdot (O/M)_{U_3O_8}$	$w_{U_3O_8} = 0/3000 * 1.179$	0.00000
f-NpO2	0.00000	$w_{NpO_2} = m_{Np}/m \cdot (O/M)_{NpO_2}$	$w_{NpO_2} = 0/3000 * 1.135$	0.00000
f-ActOx	0.7579	$w_{ActOx} = w_{PuO_2} + w_{U_3O_8} + w_{AmO_2} + w_{NpO_2}$	$w_{ActOx} = 0.756 + 0.000 + 0.00167 + 0.000$	0.7579
n-H2	0.184	$\eta_{H_2} = \begin{cases} 0.13 & (wt\%_{H_2O} \leq 0.31) \\ 0.60 \cdot 100 \cdot w_{H_2O} - 0.056 & (wt\%_{H_2O} > 0.31) \end{cases}$	$wt\%_{H_2O} = 0.4000$ $\eta_{H_2} = 0.60 \cdot 100 \cdot 0.004 - 0.056$	0.184
date dif	18.00		date diff $= (44197 - 37622)/365.25$	18.00 y
f-T-S	0.7619	$w_{T-S} = w_{ActOx} + w_{H_2O}$	$w_{T-S} = 0.7579 + 0.004$	0.7619
f-Salt	0.238	$w_S = \begin{cases} 1 - w_{T-S} & (w_{T-S} < 1.00) \\ 0 & (w_{T-S} \geq 1.00) \end{cases}$	$w_S = 1 - 0.7619$	0.238
Best_Density	6.06	$w_{T-S} < 1.00$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}} + \dfrac{w_{salt}}{\rho_{salt}}}$ $0.0 < w_{T-S} - 1 < 0.02$ OR $w_{T-S} - 1 \geq 0.02 \ \ AND \ \ w_{T-S} - 1 \geq w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}/w_{T-S}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}/w_{T-S}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}/w_{T-S}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}/w_{T-S}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}/w_{T-S}}{\rho_{H_2O}}}$ $w_{T-S} - 1 \geq 0.02 \ \ AND \ \ w_{T-S} - 1 < w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8} - (w_{T-S} - 1)}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}}}$	$w_{T-S} = 0.7619$ $\rho = 1/\left(\dfrac{0.756}{11.5} + \dfrac{0.000}{8.38} + \dfrac{0.000}{11.1} + \dfrac{0.00189}{11.7} + \dfrac{0.004}{1} + \dfrac{0.238}{2.5} \right)$	6.06 g/cm^3

Calculation Example 1: Density Condition 1 continued (3).

Density	5.450	$\rho = \rho_{test} \cdot 0.9$	$\rho = 6.06 \cdot 0.9$	5.450 g/cm³
VolInnerCont	1.879	Input variable	Input variable	1.879 L
VolOuterCont	2.155	Input variable	Input variable	2.155 L
V-GasI	1.329	$V_g = V_{U,IC} - \dfrac{m}{\rho}$	$V_g = 1.879 - \dfrac{3000}{(5.45 \cdot 1000)}$	1.329 L
Vmat	0.550	$V_m = \dfrac{m}{\rho}$	$V_m = \dfrac{3000}{(5.45 \cdot 1000)}$	0.550 L
AtmosPress_kPa_@298K	99.000	Input variable	Input variable	99.000 kPa
A	114.28	$A = P_0 \dfrac{T_1}{T_0}$	$A = 99 \cdot \dfrac{344}{298}$	114.28 kPa
B	263.85	$B = \eta_{H_2} \dfrac{m \cdot w_{H_2O}}{M_{H_2O}} \cdot \dfrac{RT_1}{V_g}$	$B = 0.182 \cdot \dfrac{3000 \cdot 0.004}{18.0152} \cdot \dfrac{8.314 \cdot 341}{1.329}$	263.85 kPa
C	12.08	$C = \eta_{He} \cdot 6.232 \times 10^{-5} \left[\dfrac{mol}{yr \cdot W}\right] \cdot \dfrac{QtRT_1}{V_g}$	$C = 0.5 \cdot 6.232 \times 10^{-5} \cdot \dfrac{10 \cdot 18 \cdot 8.314 \cdot 341}{1.329}$	12.08 kPa
TAP_IC_kPa	390.21	$P_{IC} = A + B + C$	$P_{IC} - 114.28 + 263.85 + 12.08$	390.21 kPa
TAP_OC_kPa	354.87	$P_{OC} = \dfrac{P_F(V_{U,OC} - V_{U,IC}) + P_{IC}V_{U,IC}}{V_{U,OC}}$	$P_{OC} - \dfrac{114.28 \cdot (2.155 - 1.879) + 390.21 \cdot 1.879}{2.155}$	354.87 kPa

Calculation Example 2: Density Condition 2

3013ContainerID	TEST04A

Date of Evaluation	01-Jan-21	Input variable	Input variable	01-Jan-21
Date of Evaluation (numeric)	44197.00	Input variable	Input variable	44197.00
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03
InnerCanDateTimeofweld (numeric)	37622.00	Input variable	Input variable	37622.00
3013ContainerID	TEST04A	Input variable	Input variable	TEST04A
SiteID	SRS	Input variable	Input variable	SRS
Wattage	10.00	Input variable	Input variable	10.00 W
Pu Measured (g)	2000.00	Input variable	Input variable	2000.00 g
U Measured (g)	625.00	Input variable	Input variable	625.00 g
Np Measured (g)	0.00	Input variable	Input variable	0.00 g
Am Measured (g)	0.00	Input variable	Input variable	0.00 g
MoisturePercent	0.0400	Input variable	Input variable	0.0400 wt.%
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03
ConvCanNet	3000.00	Input variable	Input variable	3000.00 g
T	344.000	$T_1 = 3Q + 1.6Q + 25 + 273$	$T_1 = 3 \cdot 10 + 1.6 \cdot 10 + 25 + 273$	344.000 K
f-H2O	0.00040	$w_{H_2O} = (wt\%_{H_2O})/100$	$w_{H_2O} = (0.0400)/100$	0.00040
f-Pu	0.667	$w_{Pu} = m_{Pu}/m$	$w_{Pu} = 2000/3000$	0.667
f-Am	0.00000	$w_{Am} = m_{Am}/m$	$w_{Am} = 0/3000$	0.00000
f-U	0.20833	$w_U = m_U/m$	$w_U = 625/3000$	0.20833
f-Np	0.00000	$w_{Np} = m_{Np}/m$	$w_{Np} = 0/3000$	0.00000

Calculation Example 2: Density Condition 2 continued (2).

f-PuO2	0.756	$w_{PuO_2} = m_{Pu}/m \cdot (O/M)_{PuO_2}$	$w_{PuO_2} = 2000/3000 * 1.134$	0.756
f-AmO2	0.00000	$w_{AmO_2} = m_{Am}/m \cdot (O/M)_{AmO_2}$	$w_{AmO_2} = 0/3000.0 * 1.132$	0.00000
f-U3O8	0.24563	$w_{U_3O_8} = m_U/m \cdot (O/M)_{U_3O_8}$	$w_{U_3O_8} = 625/3000 * 1.179$	0.24563
f-NpO2	0.00000	$w_{NpO_2} = m_{Np}/m \cdot (O/M)_{NpO_2}$	$w_{NpO_2} = 0/3000 * 1.135$	0.00000
f-ActOx	1.0016	$w_{ActOx} = w_{PuO_2} + w_{U_3O_8} + w_{AmO_2} + w_{NpO_2}$	$w_{ActOx} = 0.756 + 0.24563 + 0.000 + 0.000$	1.0016
n-H2	0.130	$\eta_{H_2} = \begin{cases} 0.13 & (wt\%_{H_2O} \leq 0.31) \\ 0.60 \cdot 100 \cdot w_{H_2O} - 0.056 & (wt\%_{H_2O} > 0.31) \end{cases}$	$wt\%_{H_2O} = 0.04$ $\eta_{H_2} = 0.13$	0.130
date dif	18.00		$date\ diff = (44197 - 37622)/365.25$	18.00 y
f-T-S	1.0020	$w_{T-S} = w_{ActOx} + w_{H_2O}$	$w_{T-S} = 1.0016 + 0.0004$	1.0020
f-Salt	0.0000	$w_S = \begin{cases} 1 - w_{T-S} & (w_{T-S} < 1.00) \\ 0 & (w_{T-S} \geq 1.00) \end{cases}$	$w_S = 0$	0.0000
Best_Density	10.50	$w_{T-S} < 1.00$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}} + \dfrac{w_{salt}}{\rho_{salt}}}$ $0.0 < w_{T-S} - 1 < 0.02$ OR $w_{T-S} - 1 \geq 0.02\ \ AND\ \ w_{T-S} - 1 \geq w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}/w_{T-S}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}/w_{T-S}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}/w_{T-S}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}/w_{T-S}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}/w_{T-S}}{\rho_{H_2O}}}$ $w_{T-S} - 1 \geq 0.02\ \ AND\ \ w_{T-S} - 1 < w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8} - (w_{T-S} - 1)}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}}}$	$w_{T-S} = 1.0020$ $\rho = 1 / \left(\dfrac{0.756/1.0008}{11.5} + \dfrac{0.24563/1.0008}{8.38} + \dfrac{0.000/1.0008}{11.1} + \dfrac{0.000/1.0008}{11.7} + \dfrac{0.0004/1.0008}{1} \right)$	10.50 g/cm³

Calculation Example 2: Density Condition 2 continued (3).

Density	9.45	$\rho = \rho_{theo} \cdot 0.9$	$\rho = 10.50 \cdot 0.9$	9.45	g/cm^3
VolInnerCont	1.972	Input variable	Input variable	1.972	L
VolOuterCont	2.248	Input variable	Input variable	2.248	L
V-GasI	1.654	$V_g = V_{U,IC} - \dfrac{m}{\rho}$	$V_g = 1.972 - \dfrac{3000}{(9.45 \cdot 1000)}$	1.654	L
Vmat	0.318	$V_m = \dfrac{m}{\rho}$	$V_m = \dfrac{3000}{(9.45 \cdot 1000)}$	0.318	L
AtmosPress_kPa_@298K	101.000	Input variable	Input variable	101.000	kPa
A	116.59	$A = P_0 \dfrac{T_1}{T_0}$	$A = 101 \cdot \dfrac{341}{298}$	116.59	kPa
B	14.97	$B = \eta_{H_2} \dfrac{m \cdot w_{H_2O}}{M_{H_2O}} \cdot \dfrac{RT_1}{V_g}$	$B = 0.13 \cdot \dfrac{3000 \cdot 0.0004}{18.0152} \cdot \dfrac{8.314 \cdot 341}{1.654}$	14.97	kPa
C	9.70	$C = \eta_{He} \cdot 6.232 \times 10^{-5} \left[\dfrac{mol}{yr \cdot W} \right] \cdot \dfrac{QtRT_1}{V_g}$	$C = 0.5 \cdot 6.232 \times 10^{-5} \cdot \dfrac{10 \cdot 18 \cdot 8.314 \cdot 341}{1.654}$	9.70	kPa
TAP_IC_kPa	141.26	$P_{IC} = A + B + C$	$P_{IC} = 116.59 + 14.97 + 9.70$	141.26	kPa
TAP_OC_kPa	138.23	$P_{OC} = \dfrac{P_F(V_{U,OC} - V_{U,IC}) + P_{IC}V_{U,IC}}{V_{U,OC}}$	$P_{OC} = \dfrac{116.59 \cdot (2.248 - 1.972) + 141.26 \cdot 1.972}{2.248}$	138.23	kPa

Calculation Example 3: Density Condition 3

3013ContainerID	TEST04B

		Input variable	Input variable		
Date of Evaluation	01-Jan-21	Input variable	Input variable	01-Jan-21	
Date of Evaluation (numeric)	44197.00	Input variable	Input variable	44197.00	
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
InnerCanDateTimeofweld (numeric)	37622.00	Input variable	Input variable	37622.00	
3013ContainerID	TEST04B	Input variable	Input variable	TEST04B	
SiteID	RFETS	Input variable	Input variable	RFETS	
Wattage	10.00	Input variable	Input variable	10.00	W
Pu Measured (g)	1000.00	Input variable	Input variable	1000.00	g
U Measured (g)	2000.00	Input variable	Input variable	2000.00	g
Np Measured (g)	0.00	Input variable	Input variable	0.00	g
Am Measured (g)	20.00	Input variable	Input variable	20.00	g
MoisturePercent	0.0600	Input variable	Input variable	0.0600	wt.%
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
ConvCanNet	3000.00	Input variable	Input variable	3000.00	g
T	344.000	$T_1 = 3Q + 1.6Q + 25 + 273$	$T_1 = 3 \cdot 10 + 1.6 \cdot 10 + 25 + 273$	344.000	K
f-H2O	0.00060	$w_{H_2O} = (wt\%_{H_2O})/100$	$w_{H_2O} = (0.06)/100$	0.00060	
f-Pu	0.333	$w_{Pu} = m_{Pu}/m$	$w_{Pu} = 1000/3000$	0.333	
f-Am	0.00667	$w_{Am} = m_{Am}/m$	$w_{Am} = 20/3000$	0.00667	
f-U	0.66667	$w_U = m_U/m$	$w_U = 2000/3000$	0.66667	
f-Np	0.00000	$w_{Np} = m_{Np}/m$	$w_{Np} = 0/3000$	0.00000	

Calculation Example 3: Density Condition 3 continued (2).

f-PuO2	0.378	$w_{PuO_2} = m_{Pu}/m \cdot (O/M)_{PuO_2}$	$w_{PuO_2} = 1000/3000 * 1.134$	0.378	
f-AmO2	0.00755	$w_{AmO_2} = m_{Am}/m \cdot (O/M)_{AmO_2}$	$w_{AmO_2} = 20/3000 * 1.132$	0.00755	
f-U3O8	0.78600	$w_{U_3O_8} = m_U/m \cdot (O/M)_{U_3O_8}$	$w_{U_3O_8} = 2000/3000 * 1.179$	0.78600	
f-NpO2	0.00000	$w_{NpO_2} = m_{Np}/m \cdot (O/M)_{NpO_2}$	$w_{NpO_2} = 0/3000 * 1.135$	0.00000	
f-ActOx	1.172	$w_{ActOx} = w_{PuO_2} + w_{U_3O_8} + w_{AmO_2} + w_{NpO_2}$	$w_{ActOx} = 0.378 + 0.786 + 0.00755 + 0.000$	1.172	
n-H2	0.130	$\eta_{H_2} = \begin{cases} 0.13 & (wt\%_{H_2O} \le 0.31) \\ 0.60 \cdot 100 \cdot w_{H_2O} - 0.056 & (wt\%_{H_2O} > 0.31) \end{cases}$	$wt\%_{H_2O} = 0.06$ $\eta_{H_2} = 0.13$	0.130	
date dif	18.00		date diff $= (44197 - 37622)/365.25$	18.00	y
f-T-S	1.172	$w_{T-S} = w_{ActOx} + w_{H_2O}$	$w_{T-S} = 1.172 + 0.0006$	1.172	
f-Salt	0.000	$w_S = \begin{cases} 1 - w_{T-S} & (w_{T-S} < 1.00) \\ 0 & (w_{T-S} \ge 1.00) \end{cases}$	$w_S = 0$	0.000	
Best_Density	9.314	$w_{T-S} < 1.00$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}} + \dfrac{w_{salt}}{\rho_{salt}}}$ $0.0 < w_{T-S} - 1 < 0.02$ OR $w_{T-S} - 1 \ge 0.02 \;\; AND \;\; w_{T-S} - 1 \ge w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}/w_{T-S}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8}/w_{T-S}}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}/w_{T-S}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}/w_{T-S}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}/w_{T-S}}{\rho_{H_2O}}}$ $w_{T-S} - 1 \ge 0.02 \;\; AND \;\; w_{T-S} - 1 < w_{U_3O_8}$ $\rho = \dfrac{1}{\dfrac{w_{PuO_2}}{\rho_{PuO_2}} + \dfrac{w_{U_3O_8} - (w_{T-S} - 1)}{\rho_{U_3O_8}} + \dfrac{w_{NpO_2}}{\rho_{NpO_2}} + \dfrac{w_{AmO_2}}{\rho_{AmO_2}} + \dfrac{w_{H_2O}}{\rho_{H_2O}}}$	$w_{T-S} = 1.172$ $\rho = 1 / \left(\dfrac{0.378}{11.5} + \dfrac{0.786 - (1.172 - 1)}{8.38} + \dfrac{0.000}{11.1} + \dfrac{0.00755}{11.7} + \dfrac{0.0006}{1} \right)$	9.314	g/cm³

Calculation Example 3: Density Condition 3 continued (3).

Density	8.382	$\rho = \rho_{best} \cdot 0.9$	$\rho = 9.314 \cdot 0.9$	8.382	g/cm^3
VolInnerCont	1.934	Input variable	Input variable	1.934	L
VolOuterCont	2.168	Input variable	Input variable	2.168	L
V-GasI	1.576	$V_g = V_{U,IC} - m/\rho$	$V_g = 1.934 - 3000/(8.382 \cdot 1000)$	1.576	L
Vmat	0.358	$V_m = m/\rho$	$V_m = 3000/(8.382 \cdot 1000)$	0.358	L
AtmosPress_kPa_@298K	81.000	Input variable	Input variable	81.000	kPa
A	93.50	$A = P_0 \dfrac{T_1}{T_0}$	$A = 81 \cdot 341/298$	93.50	kPa
B	23.57	$B = \eta_{H_2} \dfrac{m \cdot w_{H_2O}}{M_{H_2O}} \cdot \dfrac{RT_1}{V_g}$	$B = 0.13 \cdot \dfrac{3000 \cdot 0.0006}{18.0152} \cdot \dfrac{8.314 \cdot 341}{1.576}$	23.57	kPa
C	10.18	$C = \eta_{He} \cdot 6.232 \times 10^{-5} \left[\dfrac{mol}{yr \cdot W}\right] \cdot \dfrac{QtRT_1}{V_g}$	$C = 0.5 \cdot 6.232 \times 10^{-5} \cdot \dfrac{10 \cdot 18 \cdot 8.314 \cdot 341}{1.576}$	10.18	kPa
TAP_IC_kPa	127.25	$P_{IC} = A + B + C$	$P_{IC} = 93.50 + 23.57 + 10.18$	127.25	kPa
TAP_OC_kPa	123.61	$P_{OC} = \dfrac{P_F(V_{U,OC} - V_{U,IC}) + P_{IC}V_{U,IC}}{V_{U,OC}}$	$P_{OC} = \dfrac{93.50 \cdot (2.168 - 1.934) + 127.25 \cdot 1.934}{2.168}$	123.61	kPa

Calculation Example 4: Density Condition 4

3013ContainerID	TEST04A-1

Date of Evaluation	01-Jan-21	Input variable	Input variable	01-Jan-21	
Date of Evaluation (numeric)	44197.00	Input variable	Input variable	44197.00	
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
InnerCanDateTimeofweld (numeric)	37622.00	Input variable	Input variable	37622.00	
3013ContainerID	TEST04A-1	Input variable	Input variable	TEST04A-1	
SiteID	RFETS	Input variable	Input variable	RFETS	
Wattage	10.00	Input variable	Input variable	10.00	W
Pu Measured (g)	2800.00	Input variable	Input variable	2800.00	g
U Measured (g)	20.00	Input variable	Input variable	20.00	g
Np Measured (g)	0.00	Input variable	Input variable	0.00	g
Am Measured (g)	1.00	Input variable	Input variable	1.00	g
MoisturePercent	0.1000	Input variable	Input variable	0.1000	wt.%
InnerCanDateTimeofweld	01-Jan-03	Input variable	Input variable	01-Jan-03	
ConvCanNet	3000.00	Input variable	Input variable	3000.00	g
T	344.000	$T_1 = 3Q + 1.6Q + 25 + 273$	$T_1 = 3 \cdot 10 + 1.6 \cdot 10 + 25 + 273$	344.000	K
f-H2O	0.00100	$w_{H2O} = (wt\%_{H_2O})/100$	$w_{H2O} = (0.1)/100$	0.00100	
f-Pu	0.933	$w_{Pu} = m_{Pu}/m$	$w_{Pu} = 2800/3000$	0.933	
f-Am	0.00033	$w_{Am} = m_{Am}/m$	$w_{Am} = 1/3000$	0.00033	
f-U	0.00667	$w_U = m_U/m$	$w_U = 20/3000$	0.00667	
f-Np	0.00000	$w_{Np} = m_{Np}/m$	$w_{Np} = 0/3000$	0.00000	

Calculation Example 4: Density Condition 4 continued (2).

f-PuO2	1.058	$w_{PuO_2} = m_{Pu}/m \cdot (O/M)_{PuO_2}$	$w_{PuO_2} = 2800/3000 * 1.134$	1.058	
f-AmO2	0.00038	$w_{AmO_2} = m_{Am}/m \cdot (O/M)_{AmO_2}$	$w_{AmO_2} = 1/3000 * 1.132$	0.00038	
f-U3O8	0.00786	$w_{U_3O_8} = m_U/m \cdot (O/M)_{U_3O_8}$	$w_{U_3O_8} = 20/3000 * 1.179$	0.00786	
f-NpO2	0.00000	$w_{NpO_2} = m_{Np}/m \cdot (O/M)_{NpO_2}$	$w_{NpO_2} = 0/3000 * 1.135$	0.00000	
f-ActOx	1.0666	$w_{ActOx} = w_{PuO_2} + w_{U_3O_8} + w_{AmO_2} + w_{NpO_2}$	$w_{ActOx} = 1.058 + 0.00786 + 0.00038 + 0.000$	1.0666	
n-H2	0.130	$\eta_{H_2} = \begin{cases} 0.13 & (wt\%_{H_2O} \le 0.31) \\ 0.60 \cdot 100 \cdot w_{H_2O} - 0.056 & (wt\%_{H_2O} > 0.31) \end{cases}$	$wt\%_{H_2O} = 0.1$ $\eta_{H_2} = 0.13$	0.130	
date dif	18.00		$\text{date diff} = (44197 - 37622)/365.25$	18.00	y
f-T-S	1.0676	$w_{T-S} = w_{ActOx} + w_{H_2O}$	$w_{T-S} = 1.0666 + 0.001$	1.0676	
f-Salt	0.0000	$w_S = \begin{cases} 1 - w_{T-S} & (w_{T-S} < 1.00) \\ 0 & (w_{T-S} \ge 1.00) \end{cases}$	$w_S = 0$	0.0000	
Best_Density	11.357	$w_{T-S} < 1.00$ $\rho = \dfrac{1}{\frac{w_{PuO_2}}{\rho_{PuO_2}} + \frac{w_{U_3O_8}}{\rho_{U_3O_8}} + \frac{w_{NpO_2}}{\rho_{NpO_2}} + \frac{w_{AmO_2}}{\rho_{AmO_2}} + \frac{w_{H_2O}}{\rho_{H_2O}} + \frac{w_{salt}}{\rho_{salt}}}$ $0.0 < w_{T-S} - 1 < 0.02$ OR $w_{T-S} - 1 \ge 0.02 \ \ AND \ \ w_{T-S} - 1 \ge w_{U_3O_8}$ $\rho = \dfrac{1}{\frac{w_{PuO_2}/w_{T-S}}{\rho_{PuO_2}} + \frac{w_{U_3O_8}/w_{T-S}}{\rho_{U_3O_8}} + \frac{w_{NpO_2}/w_{T-S}}{\rho_{NpO_2}} + \frac{w_{AmO_2}/w_{T-S}}{\rho_{AmO_2}} + \frac{w_{H_2O}/w_{T-S}}{\rho_{H_2O}}}$ $w_{T-S} - 1 \ge 0.02 \ \ AND \ \ w_{T-S} - 1 < w_{U_3O_8}$ $\rho = \dfrac{1}{\frac{w_{PuO_2}}{\rho_{PuO_2}} + \frac{w_{U_3O_8} - (w_{T-S} - 1)}{\rho_{U_3O_8}} + \frac{w_{NpO_2}}{\rho_{NpO_2}} + \frac{w_{AmO_2}}{\rho_{AmO_2}} + \frac{w_{H_2O}}{\rho_{H_2O}}}$	$w_{T-S} = 1.0676 \qquad w_{T-S} - 1 = 0.0676$ $w_{U_3O_8} = 0.00786$ $\rho = 1 \Big/ \left(\frac{1.058/1.0676}{11.5} + \frac{0.00786/1.0676}{8.38} + \frac{0.000/1.0676}{11.1} + \frac{0.00038/1.0676}{11.7} + \frac{0.001/1.0676}{1} \right)$	11.357	g/cm³

Calculation Example 4: Density Condition 4 continued (3).

Density	10.222	$\rho = \rho_{best} \cdot 0.9$	$\rho = 11.357 \cdot 0.9$	10.222 g/cm^3
VolInnerCont	1.934	Input variable	Input variable	1.934 L
VolOuterCont	2.168	Input variable	Input variable	2.168 L
V-GasI	1.641	$V_g = V_{U,IC} - \dfrac{m}{\rho}$	$V_g = 1.934 - \dfrac{3000}{(10.222 \cdot 1000)}$	1.641 L
Vmat	0.293	$V_m = \dfrac{m}{\rho}$	$V_m = \dfrac{3000}{(10.222 \cdot 1000)}$	0.293 L
AtmosPress_kPa_@298K	81.000	Input variable	Input variable	81.000 kPa
A	93.50	$A = P_0 \dfrac{T_1}{T_0}$	$A = 81 \cdot \dfrac{341}{298}$	93.50 kPa
B	37.74	$B = \eta_{H_2} \dfrac{m \cdot w_{H_2O}}{M_{H_2O}} \cdot \dfrac{RT_1}{V_g}$	$B = 0.13 \cdot \dfrac{3000 \cdot 0.001}{18.0152} \cdot \dfrac{8.314 \cdot 341}{1.641}$	37.74 kPa
C	9.78	$C = \eta_{He} \cdot 6.232 \times 10^{-5} \left[\dfrac{mol}{yr \cdot W} \right] \cdot \dfrac{QtRT_1}{V_g}$	$C = 0.5 \cdot 6.232 \times 10^{-5} \cdot \dfrac{10 \cdot 18 \cdot 8.314 \cdot 341}{1.641}$	9.78 kPa
TAP_IC_kPa	141.02	$P_{IC} = A + B + C$	$P_{IC} = 93.50 + 37.74 + 9.78$	141.02 kPa
TAP_OC_kPa	135.89	$P_{OC} = \dfrac{P_E (V_{U,OC} - V_{U,IC}) + P_{IC} V_{U,IC}}{V_{U,OC}}$	$P_{OC} = \dfrac{93.50 \cdot (2.168 - 1.934) + 141.02 \cdot 1.934}{2.168}$	135.89 kPa

Appendix 2.
Comparison of Calculated Container Pressure and Pressure Measured by Destructive Evaluation

Table 8. Comparison of the Pressures Measured at the Time of Destructive Evaluation (DE) with the Calculated Pressures Obtained Using the 2018 and 2008 Versions of the ISP Database Pressure Equation[1].

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	[2]ΔT for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2007	1	R600885	RFETS	27-Feb-02	17-Jun-07	18.8	88.3	165.7	143.5	143.7	463.3
2007	2	R601722	RFETS	20-Feb-02	03-Jul-07	18.9	86.2	218.4	144.0	144.2	452.1
2007	3	R601957	RFETS	19-Feb-02	18-Jul-07	18.9	88.3	117.0	141.7	141.7	484.5
2007	4	R600719	RFETS	14-Jan-02	26-Jul-07	19.0	88.9	165.8	142.7	171.8	210.2
2007	5	R610735	RFETS	14-May-03	06-Aug-07	17.6	85.5	222.5	136.1	167.4	248.7
2007	6	R610697	RFETS	16-May-03	14-Aug-07	17.6	86.2	192.8	137.4	175.9	236.1
2007	7	R601285	RFETS	14-May-02	28-Aug-07	18.6	92.4	208.6	145.3	145.5	442.3
2008	1	R602731	RFETS	10-Oct-02	13-Nov-07	18.2	84.8	122.2	137.3	146.6	266.2
2008	2	R601318	RFETS	20-May-02	28-Nov-07	18.6	86.9	190.7	142.6	142.8	467.3
2008	3	H000898	RFETS	18-Dec-02	11-Dec-07	18.0	84.8	101.6	141.3	141.3	442.8
2008	4	R610327	RFETS	02-Jan-03	14-Jan-08	18.0	85.5	85.3	132.7	132.8	345.6
2008	5	R610298	RFETS	13-Jan-03	30-Jan-08	18.0	89.6	98.8	138.7	139.4	207.8
2008	6	R610324	RFETS	26-Feb-03	12-Feb-08	17.8	90.3	97.3	137.7	139.3	229.8
2008	7	H001992	Hanford	11-Sep-02	26-Feb-08	18.3	91.7	153.0	156.5	156.5	415.5
2008	8	H003157	Hanford	21-Oct-02	12-Mar-08	18.2	85.5	162.7	172.0	172.7	390.1
2008	9	R610584	RFETS	07-Apr-03	07-Apr-08	17.7	94.5	166.6	139.7	139.8	457.0
2008	10	R610578	RFETS	08-Apr-03	17-Apr-08	17.7	86.2	106.2	138.4	141.9	211.3
2008	11	H001916	Hanford	22-Aug-02	06-May-08	18.4	91.7	103.5	151.6	151.6	526.6
2008	12	H002088	Hanford	06-Nov-02	21-May-08	18.2	85.5	144.4	167.1	167.9	392.1

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	$^2\Delta T$ for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2008	13	H003409	Hanford	24-Jun-03	04-Jun-08	17.5	92.4	177.5	156.2	184.3	235.7
2008	14	H002573	Hanford	08-Jul-03	08-Jul-08	17.5	121.4	197.6	156.2	191.7	238.9
2008	15	H002534	Hanford	14-Jul-03	23-Jul-08	17.5	94.5	190.9	156.0	186.9	237.4
2008	16	R610679	RFETS	18-Apr-03	05-Aug-08	17.7	80.7	129.8	140.0	140.0	406.4
2008	17	H002750	Hanford	08-Jul-03	19-Aug-08	17.5	90.3	120.0	157.9	160.1	215.3
2009	1	H004099	Hanford	26-Nov-03	10-Sep-08	17.1	80.7	215.3	161.7	161.9	457.5
2009	2	H004111	Hanford	03-Dec-03	30-Sep-08	17.1	99.3	201.8	156.2	192.5	237.0
2009	3	H002554	Hanford	24-Jul-03	05-Nov-08	17.4	85.5	188.7	156.0	186.3	236.9
2009	4	H001941	Hanford	01-Oct-02	18-Nov-08	18.3	91.0	116.4	157.4	157.4	446.2
2009	5	R602498	RFETS	08-Oct-02	09-Dec-08	18.2	84.8	212.1	140.0	194.3	220.4
2009	6	H002509	Hanford	27-Jul-03	21-Jan-09	17.4	142.0	209.9	156.1	194.7	236.5
2009	7	H002565	Hanford	27-Jul-03	03-Feb-09	17.4	76.5	205.1	156.1	192.5	236.7
2009	8	H002657	Hanford	10-Jul-03	17-Feb-09	17.5	77.2	165.3	156.3	180.2	237.5
2009	9	R611398	RFETS	02-Jul-03	10-Mar-09	17.5	78.6	231.5	139.8	139.9	467.2
2009	10	H002200	Hanford	04-Feb-03	24-Mar-09	17.9	93.1	134.5	160.9	160.9	411.0
2009	11	H002667	Hanford	15-Jul-03	06-Apr-09	17.5	80.0	154.9	155.5	174.0	241.0
2009	12	H002715	Hanford	05-Aug-03	23-Apr-09	17.4	141.3	210.5	156.1	194.7	237.3
2009	13	R610700	RFETS	18-Apr-03	05-May-09	17.7	79.3	122.1	140.6	140.6	378.2
2009	14	R610764	RFETS	22-Apr-03	27-May-09	17.7	84.1	99.2	134.9	139.1	257.0
2009	15	R610573	RFETS	15-Apr-03	10-Jun-09	17.7	94.5	138.0	136.9	152.6	232.1
2009	16	R610558	RFETS	14-Apr-03	08-Jul-09	17.7	84.8	100.1	141.6	141.6	482.9
2009	17	R610806	RFETS	16-Apr-03	21-Jul-09	17.7	84.1	173.0	141.4	168.9	203.2
2009	18	H003119	Hanford	19-Jan-04	05-Aug-09	17.0	80.7	143.8	157.5	172.8	216.4
2009	19	H002195	Hanford	03-Feb-03	18-Aug-09	17.9	94.5	122.4	162.4	162.4	440.6
2010	1	H004251	Hanford	10-Dec-03	23-Sep-09	17.1	120.7	174.2	155.4	174.5	234.1
2010	2	H002496	Hanford	27-Jul-03	07-Oct-09	17.4	80.0	156.2	153.5	167.8	258.9

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	$^2\Delta T$ for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2010	3	H003710	Hanford	04-Sep-03	27-Oct-09	17.3	114.5	231.8	156.4	200.2	235.8
2010	4	H003655	Hanford	27-Aug-03	10-Nov-09	17.3	121.4	198.4	156.4	190.6	234.1
2010	5	H002447	Hanford	12-May-03	03-Dec-09	17.6	82.7	122.4	156.3	161.7	235.4
2010	6	R610627	RFETS	13-May-03	05-Jan-10	17.6	101.4	100.5	136.6	138.7	217.1
2010	7	H003900	Hanford	30-Oct-03	20-Jan-10	17.2	117.2	212.8	155.6	187.6	238.7
2010	8	H003650	Hanford	03-Sep-03	02-Feb-10	17.3	88.3	202.4	156.5	196.0	235.7
2010	9	H002567	Hanford	23-Jul-03	17-Feb-10	17.4	80.7	105.7	150.9	152.4	285.3
2010	10	H002728	Hanford	25-Jun-03	11-Mar-10	17.5	78.6†	162.2	155.9	176.6	236.8
2010	11	H002786	Hanford	09-Jul-03	09-Apr-10	17.5	86.2	189.9	156.0	187.0	238.4
2010	12	H003077	Hanford	05-Jun-03	22-Apr-10	17.6	84.1	155.6	159.6	177.4	218.5
2010	13	H003367	Hanford	18-Jun-03	06-May-10	17.5	79.3	142.1	153.6	163.5	254.1
2010	14	H003704	Hanford	21-Sep-03	04-Jun-10	17.3	105.5	201.9	156.3	192.8	234.1
2010	15	R610785	RFETS	30-Apr-03	15-Jun-10	17.7	95.8	97.1	136.9	138.4	225.9
2010	16	R610826	RFETS	13-May-03	08-Jul-10	17.6	82.7	97.1	136.9	138.0	213.2
2010	17	R610853	RFETS	12-May-03	22-Jul-10	17.6	84.8	114.5	140.0	145.8	207.9
2010	18	S001721	SRS	28-May-04	06-Aug-10	16.6	82.7	221.9	164.3	210.8	229.4
2011	1	H003443	Hanford	22-Jul-03	26-Aug-10	17.4	124.8	206.6	156.0	192.7	237.2
2011	2	S002129	SRS	20-Oct-04	21-Sep-10	16.2	85.5	295.7	166.6	235.3	214.3
2011	3	H002592	Hanford	31-Jul-03	30-Sep-10	17.4	81.4	108.4	151.9	153.4	275.4
2011	4	H003337	Hanford	12-Oct-03	19-Oct-10	17.2	84.8	144.6	154.4	164.9	244.3
2011	5	S001105	SRS	18-Oct-04	04-Nov-10	16.2	82.7	266.8	166.6	223.6	215.6
2011	6	H003343	Hanford	03-Oct-03	30-Nov-10	17.2	80.0	146.8	154.7	172.7	245.7
2011	7	H003371	Hanford	18-Jun-03	05-Jan-11	17.5	83.4	161.4	154.0	154.1	508.0
2011	8	H003526	Hanford	25-Aug-03	24-Jan-11	17.4	69.0	152.6	155.8	172.2	237.2
2011	9	H003565	Hanford	07-Sep-03	03-Feb-11	17.3	72.4	160.1	156.3	177.7	235.6
2011	10	R611131	RFETS	03-Jun-03	01-Mar-11	17.6	95.2	103.8	139.8	142.8	219.8

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	$^2\Delta T$ for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2011	11	H003625	Hanford	03-Sep-03	17-Mar-11	17.3	81.4	155.0	156.2	174.9	234.7
2011	12	L000178	LLNL	23-Jul-03	14-Jun-11	17.4	95.2	107.5	153.5	153.6	237.2
2011	13	H003328	Hanford	30-Sep-03	13-Sep-10	17.3	299.2[†]	430.5	157.1	230.9	229.8
2012	1	H001209	Hanford	23-May-02	21-Sep-11	18.6	83.4	125.2	150.9	151.0	620.7
2012	2	H002574	Hanford	19-Jun-03	12-Oct-11	17.5	88.3	140.5	152.9	152.9	530.9
2012	3	H001513	Hanford	15-Jul-02	07-Nov-11	18.5	77.9	129.3	151.1	151.1	616.8
2012	4	H003390	Hanford	18-Jun-03	08-Dec-11	17.5	78.6	167.0	156.6	172.2	218.9
2012	5	L000075	LLNL	16-Jan-03	09-Jan-12	18.0	97.9	126.5	163.9	164.1	193.1
2012	5	L000075	LLNL	16-Jan-03	09-Jan-12	18.0	97.9	126.5	163.9	164.1	189.1
2012	5	L000075	LLNL	16-Jan-03	09-Jan-12	18.0	97.9	126.9	163.9	164.1	193.1
2012	5	L000075	LLNL	16-Jan-03	09-Jan-12	18.0	97.9	126.9	163.9	164.1	189.1
2012	6	H004012	Hanford	05-Nov-03	31-Jan-12	17.2	75.2	157.9	155.3	171.4	238.1
2012	7	H004048	Hanford	04-Nov-03	01-Mar-12	17.2	67.6	142.4	154.5	164.2	241.8
2012	8	R610960	RFETS	15-May-03	03-May-12	17.6	89.6	107.6	136.9	141.4	224.6
2012	10	S002250	SRS	08-Jan-05	15-Mar-12	16.0	93.8	139.6	161.6	161.6	415.3
2013	1	H001236	Hanford	23-Apr-02	22-Apr-13	18.7	85.5	147.0	150.5	150.6	634.0
2014	1	R610996	RFETS	15-May-03	15-Jan-14	17.6	84.1	103.1	137.8	139.5	187.4
2014	2	H003064	Hanford	08-Jan-04	04-Feb-14	17.0	157.9	208.0	156.0	192.2	237.4
2014	3	H003307	Hanford	10-Dec-03	20-Feb-14	17.1	77.2	158.4	155.1	173.4	241.8
2014	4	H003052	Hanford	29-Dec-03	27-Mar-14	17.0	71.7	175.2	155.8	179.4	234.2
2014	5	H003898	Hanford	28-Oct-03	09-Apr-14	17.2	80.7	162.0	155.5	173.9	238.0
2014	6	S002277	SRS	25-Oct-04	24-Apr-14	16.2	84.1	282.0	166.5	230.3	218.0
2014	7	S002116	SRS	13-Nov-04	08-May-14	16.1	89.6	218.0	166.1	203.9	219.5
2014	8	H004219	Hanford	14-Dec-03	21-May-14	17.1	72.4	149.1	154.5	170.1	246.9
2014	9	H002636	Hanford	29-Jun-03	02-Jun-14	17.5	84.8	126.5	163.5	163.5	443.0
2015	1	R610156	RFETS	20-Jan-03	14-Nov-14	17.9	86.2	130.9	133.6	147.2	291.0

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	$^2\Delta T$ for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2015	2	S002162	SRS	08-Nov-04	03-Dec-14	16.1	83.4	192.0	166.1	193.7	219.0
2015	3	H001979	Hanford	31-Dec-03	09-Jan-15	17.0	82.1	139.3	155.6	167.5	236.5
2015	4	H001181	Hanford	01-Apr-02	04-Feb-15	18.8	89.6	137.6	152.1	152.2	593.8
2015	5	H003181	Hanford	08-Jan-04	12-Feb-15	17.0	90.3	203.2	156.7	196.1	230.3
2015	6	H003258	Hanford	12-Jan-04	15-Apr-15	17.0	77.2	157.2	155.9	174.3	236.8
2015	7	H003737	Hanford	20-Aug-03	06-May-15	17.4	71.7	187.6	156.0	186.0	236.9
2015	8	H003896	Hanford	28-Oct-03	04-Jun-15	17.2	148.9	207.8	155.8	187.8	236.5
2015	9	H004302	Hanford	18-Jan-04	18-Jun-15	17.0	80.0	172.0	155.8	179.4	233.2
2016	1	H001191	Hanford	24-Jul-02	19-Feb-16	18.4	77.9	136.1	152.2	152.3	591.4
2016	2	H002556	Hanford	08-Jul-03	03-Mar-16	17.5	72.4	158.3	156.1	175.9	238.2
2016	3	H004173	Hanford	04-Dec-03	12-May-16	17.1	80.7	164.8	156.0	177.7	235.5
2016	4	H004247	Hanford	09-Dec-03	08-Jun-16	17.1	82.7	152.9	155.5	170.8	236.2
2016	5	H003775	Hanford	07-Oct-03	22-Jun-16	17.2	71.7	158.9	157.2	180.1	224.7
2016	6	H004024	Hanford	14-Nov-03	06-Jul-16	17.1	76.5	169.5	156.0	179.8	236.9
2017	1	H001304	Hanford	20-May-02	05-Jan-17	18.6	84.8	134.2	151.2	151.2	596.7
2017	2	H002575	Hanford	05-Aug-03	03-Feb-17	17.4	94.5	204.2	156.4	195.8	236.0
2017	3	H003352	Hanford	05-Oct-03	03-Apr-17	17.2	57.9	200.9	156.3	194.2	234.9
2017	4	H003695	Hanford	01-Sep-03	17-Apr-17	17.3	128.9	196.2	156.2	190.7	235.3
2017	5	H002508	Hanford	23-Jul-03	11-May-17	17.4	104.1	187.1	155.8	184.9	238.7
2017	6	R600793	RFETS	04-Mar-02	05-Jun-17	18.8	90.3	332.0	143.4	236.9	198.4
2018	1	H003345	Hanford	09-Oct-03	03-Oct-17	17.2	78.6	184.9	155.3	179.3	240.2
2018	2	H003626	Hanford	03-Sep-03	01-Nov-17	17.3	69.6	179.3	156.4	186.3	234.9
2018	3	H003645	Hanford	04-Sep-03	14-Nov-17	17.3	72.4	182.7	156.2	185.8	235.5
2018	4	H002524	Hanford	27-Jul-03	05-Dec-17	17.4	66.2	168.3	156.0	178.9	236.7
2018	5	H003523	Hanford	25-Aug-03	12-Dec-17	17.4	79.3	170.4	155.9	180.4	237.6
2018	6	H004153	Hanford	19-Nov-03	23-Jan-18	17.1	59.3	192.6	155.2	180.4	240.5

Surv. Year	DE No.	3013 Container ID	Packaging Site ID	3013 Inner Container Weld Date	3013 Inner Container Puncture Date	[2]ΔT for Calculation of Pressure (y)	IC Pressure Meas. at DE (kPa)	Calculated IC Pressure v. 2018 (kPa)	Calculated IC Pressure v. 2008 (kPa)	Calculated P_{max} v. 2008 (kPa)	Time to Reach P_{max} v. 2008 (d)
2019	1	A000632	LANL	01-Apr-10	13-Nov-18	10.8	72.4	111.1	141.7	152.3	223.7

[1] Pressures evaluated for January 1, 2021.

[2] Δt is the elapsed time from the date of inner container welding to the date of evaluation of the pressure (January 1, 2021).

[†] From Ref 5 Veirs, D. K.; Kelly, E. J.; Berg, J. M.; Nguyen, B. V.; McClard, J.; Hensel, S.; Duffey, J. M.; Scogin, J. H. Gas composition observed by destructive evaluation of 3013 containers; LA-UR-17-31465; Los Alamos National Laboratory: Los Alamos, NM, 2017.

Appendix 3.
SQL Code for the 2018 Version
of the ISP Database Pressure Equation

```
SELECT DISTINCT tblPCDCalGamma.[3013ContainerID], tblPCDProcessed.SiteID,
tblPCDProcessed.MISRepresented, tblPCDProcessed.FY16ISPBin,
tblPCDProcessed.FY16ISPSubBin, tblPCDInnerCan.InnerCanDateTimeofweld,
tblPCDMoisture.MoisturePercent, tblPCDMoisture.MoistureMethod,
tblPCDMoisture.StorageWeightGain,
[tblPCDCalGamma]![Wattage]*3+[tblPCDCalGamma]![Wattage]*1.6+25+273 AS T,
IIf([tblPCDMoisture]![MoisturePercent]<0,0,[tblPCDMoisture]![MoisturePercent]/100) AS [f-H2O],
Nz([Pu Measured (g)])/Nz([ConvCanNet]) AS [f-Pu], Nz([Am Measured (g)])/Nz([ConvCanNet]) AS
[f-Am], Nz([U Measured (g)])/Nz([ConvCanNet]) AS [f-U], Nz([Np Measured
(g)])/Nz([ConvCanNet]) AS [f-Np], Nz([Pu Measured (g)])/Nz([ConvCanNet])*1.134 AS [f-PuO2],
Nz([Am Measured (g)])/Nz([ConvCanNet])*1.132 AS [f-AmO2], Nz([U Measured
(g)])/Nz([ConvCanNet])*1.179 AS [f-U3O8], Nz([Np Measured (g)])/Nz([ConvCanNet])*1.135 AS [f-
NpO2], (Nz([Pu Measured (g)])/Nz([ConvCanNet]))*1.134+(Nz([U Measured
(g)])/Nz([ConvCanNet]))*1.179+(Nz([Am Measured (g)])/Nz([ConvCanNet]))*1.132+(Nz([Np
Measured (g)])/Nz([ConvCanNet]))*1.135 AS [f-ActOx],
IIf([tblPCDMoisture]![MoisturePercent]<0,0,IIf([tblPCDMoisture]![MoisturePercent]<0.31,0.13,0.6*[t
blPCDMoisture]![MoisturePercent]-0.056)) AS [n-H2], DateDiff("d",[tblPCDInnerCan
]![InnerCanDateTimeofweld],[Pressure Calculation End Date])/365.25 AS [date dif], [f-ActOx]+[f-
H2O] AS [f-T-S], IIf([f-T-S]<1,1-[f-T-S],0) AS [f-Salt], IIf([f-T-S]<1,1/(([f-PuO2]/11.5)+([f-
U3O8]/8.38)+([f-AmO2]/11.7)+([f-NpO2]/11.1)+((1-[f-T-S])/2.5)+[f-H2O]),IIf([f-T-S]-1<0.02,1/((([f-
PuO2]/[f-T-S])/11.5)+(([f-U3O8]/[f-T-S])/8.38)+(([f-AmO2]/[f-T-S])/11.7)+(([f-NpO2]/[f-T-
S])/11.1)+([f-H2O]/[f-T-S])),IIf([f-U3O8]<[f-T-S]-1,1/((([f-PuO2]/[f-T-S])/11.5)+(([f-U3O8]/[f-T-
S])/8.38)+(([f-AmO2]/[f-T-S])/11.7)+(([f-NpO2]/[f-T-S])/11.1)+([f-H2O]/[f-T-S])),1/((([f-
PuO2]/11.5)+(([f-U3O8]-([f-T-S]-1))/8.38)+([f-AmO2]/11.7)+([f-NpO2]/11.1)+[f-H2O])))) AS
Best_Density, [Best_Density]*0.9 AS Density, tblPCDProcessed.VolInnerCont,
tblPCDProcessed.VolOuterCont, [tblPCDProcessed]![VolInnerCont]-
[tblPCDConvCan]![ConvCanNet]/([Density]*1000) AS [V-GasI],
[tblPCDConvCan]![ConvCanNet]/[Density]/1000 AS Vmat, IIf([tblPCDProcessed].[SiteID]=1 Or
[tblPCDProcessed].[SiteID ]=3,99,IIf([tblPCDProcessed].[SiteID
]=2,78,IIf([tblPCDProcessed].[SiteID]=4,81,IIf([tblPCDProcessed].[SiteID]=5,101,-9999)))) AS
[AtmosPress_kPa_@298K], [AtmosPress_kPa_@298K]*[T]/298 AS A, [n-H2]*([ConvCanNet]*[f-
H2O]/18.0152)*8.314*[T]/[V-GasI] AS B, 0.5*0.00006232*[Wattage]*[date dif]*8.314*[T]/[V-GasI]
AS C, [A]+[B]+[C] AS TAP_IC_kPa, ([A]*([VolOuterCont]-
[VolInnerCont])+[TAP_IC_kPa]*[VolInnerCont])/[VolOuterCont] AS TAP_OC_kPa,
tblPCDConvCan.ConvCanNet

FROM (((tblPCDConvCan INNER JOIN tblPCDInnerCan ON (tblPCDConvCan.SiteID =
tblPCDInnerCan.SiteID) AND (tblPCDConvCan.InnerCanID = tblPCDInnerCan.InnerCanID))
INNER JOIN tblPCDMoisture ON (tblPCDConvCan.ConvCanID = tblPCDMoisture.ConvCanID)
AND (tblPCDConvCan.SiteID = tblPCDMoisture.SiteID)) INNER JOIN tblPCDCalGamma ON
tblPCDInnerCan.[3013ContainerID] = tblPCDCalGamma.[3013ContainerID]) INNER JOIN
tblPCDProcessed ON tblPCDInnerCan.[3013ContainerID] = tblPCDProcessed.[3013ContainerID]

WHERE (((tblPCDMoisture.BestMoisture)=True));
```

Appendix 4.
Modified SQL Code for the 2008 Version
of the ISP Database Pressure Equation

```
SELECT tblPCDCalGamma.[3013ContainerID], tblPCDMoisture.MoisturePercent,
tblPCDProcessed.GValue, [tblPCDCalGamma]![Wattage]/[tblPCDConvCan]![ConvCanNet]*1000
AS SA, [tblPCDCalGamma]![Wattage]*3+[tblPCDCalGamma]![Wattage]*1.6+25+273 AS T,
IIf([tblPCDMoisture]![MoisturePercent]<0,0,[tblPCDMoisture]![MoisturePercent]/100) AS [f-H2O],
Nz([Pu Measured (g)])/Nz([ConvCanNet]) AS [f-Pu], Nz([Am Measured (g)])/Nz([ConvCanNet]) AS
[f-Am], Nz([U Measured (g)])/Nz([ConvCanNet]) AS [f-U], Nz([Np Measured
(g)])/Nz([ConvCanNet]) AS [f-Np], Nz([Pu Measured (g)])/Nz([ConvCanNet])*1.134 AS [f-PuO2],
Nz([Am Measured (g)])/Nz([ConvCanNet])*1.132 AS [f-AmO2], Nz([U Measured
(g)])/Nz([ConvCanNet])*1.179 AS [f-U3O8], (Nz([Np Measured (g)]/Nz([ConvCanNet])))*1.135 AS
[f-NpO2], (Nz([Pu Measured (g)])/Nz([ConvCanNet]))*1.134+(Nz([U Measured
(g)])/Nz([ConvCanNet]))*1.179+(Nz([Am Measured (g)])/Nz([ConvCanNet]))*1.132+(Nz([Np
Measured (g)])/Nz([ConvCanNet]))*1.135 AS [f-ActOx],
IIf([tblPCDMoisture]![MoisturePercent]<0,0,[tblPCDConvCan]![ConvCanNet]*([tblPCDMoisture]![M
oisturePercent]/100)/18.0152) AS [n-H2O], DateDiff("s",[tblPCDInnerCan
]![InnerCanDateTimeofweld],[Pressure Calculation End Date]) AS [date dif], [f-ActOx]+[f-H2O] AS
[f-T-S], IIf([f-T-S]<1,1-[f-T-S],0) AS [f-Salt], IIf([f-T-S]<1,1/((([f-PuO2]/11.5)+([f-U3O8]/8.38)+([f-
AmO2]/11.7)+([f-NpO2]/11.1)+((1-[f-T-S])/2.5)+[f-H2O])),IIf([f-T-S]-1<0.02,1/(((([f-PuO2]/[f-T-
S])/11.5)+(([f-U3O8]/[f-T-S])/8.38)+(([f-AmO2]/[f-T-S])/11.7)+(([f-NpO2]/[f-T-S])/11.1)+([f-H2O]/[f-T-
S])),IIf([f-U3O8]<[f-T-S]-1,1/(((([f-PuO2]/[f-T-S])/11.5)+(([f-U3O8]/[f-T-S])/8.38)+(([f-AmO2]/[f-T-
S])/11.7)+(([f-NpO2]/[f-T-S])/11.1)+([f-H2O]/[f-T-S])),1/((([f-PuO2]/11.5)+(([f-U3O8]-([f-T-S]-
1))/8.38)+([f-AmO2]/11.7)+([f-NpO2]/11.1)+[f-H2O])))) AS Density,
[tblPCDProcessed]![VolInnerCont]-[tblPCDConvCan]![ConvCanNet]/([Density]*1000)-
[tblPCDConvCan]![ConvCanTare]/(8*1000) AS [V-Gas], (10/18)/([f-PuO2]*(110/271)+[f-
AmO2]*(111/275)+[f-U3O8]*(340/833)+[f-NpO2]*(109/269)+[f-H2O]*(10/18)+0.5*[f-Salt]) AS [f-e-
H2O], [tblPCDProcessed]![GValue]*[SA]*[f-e-H2O]*18.1052*0.000000000001 AS C,
8.3145*[T]/[V-Gas] AS [RT/V], 0.000000000075 AS k, ([C]*[RT/V]*[n-H2O])/(([k]*[RT/V])-[C]) AS A,
Exp(-[C]*[date dif])-Exp(-[k]*[RT/V]*[date dif]) AS b, [A]*[b] AS [H2 Pressure],
IIf([tblPCDProcessed].[SiteID]=1 Or [tblPCDProcessed].[SiteID
]=3,99,IIf([tblPCDProcessed].[SiteID
]=2,78,IIf([tblPCDProcessed].[SiteID]=4,81,IIf([tblPCDProcessed].[SiteID]=5,101,-9999)))) AS
AtmosPress_kPa, [AtmosPress_kPa]*[T]/298 AS AtmosPres_kPa_adjusted, [H2
Pressure]+50+[AtmosPres_kPa_adjusted] AS TotalAbsPres_kPa, [k]*[RT/V]/[C] AS Kappa, [n-
H2O]*[RT/V]*([Kappa]^([Kappa]/(1-[Kappa]))) AS PmaxH2_kPa,
[PmaxH2_kPa]+50+[AtmosPres_kPa_adjusted] AS MaxTotalAbsPres_kPa, ((Log([k]*[RT/V])-
Log([C]))/([k]*[RT/V]-[C]))/86400 AS tmax_d, [tblPCDInnerCan
]![InnerCanDateTimeofweld]+[tmax_d] AS tmax_date
FROM (tblPCDConvCan INNER JOIN (tblPCDInnerCan INNER JOIN (tblPCDProcessed INNER
JOIN tblPCDCalGamma ON (tblPCDProcessed.[3013ContainerID] =
tblPCDCalGamma.[3013ContainerID]) AND (tblPCDProcessed.SiteID =
tblPCDCalGamma.SiteID)) ON (tblPCDInnerCan.[3013ContainerID] =
tblPCDProcessed.[3013ContainerID]) AND (tblPCDInnerCan.SiteID = tblPCDProcessed.SiteID))
ON (tblPCDConvCan.InnerCanID = tblPCDInnerCan.InnerCanID) AND (tblPCDConvCan.SiteID =
tblPCDInnerCan.SiteID)) INNER JOIN tblPCDMoisture ON (tblPCDConvCan.SiteID =
tblPCDMoisture.SiteID) AND (tblPCDConvCan.ConvCanID = tblPCDMoisture.ConvCanID)
WHERE (((tblPCDMoisture.BestMoisture)=True))
ORDER BY tblPCDCalGamma.[3013ContainerID];
```

The SQL code for the 2008 Version of the ISP Database pressure equation used to compare
output is given in the box above. This version of the pressure equation includes terms for
hydrogen formation as well as consumption. Therefore, fields for calculating the maximum

pressure $P_{IC,max}$ and the time to reach maximum pressure t_{max} were added for purposes of comparison.

The model for hydrogen gas generation and consumption used in the code was a first order intermediate of the form shown in Eq. (9).

$$P_{H_2}(t) = \frac{A_0 k_1}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) \tag{9}$$

The parameters A_0, k_1, and k_2 are given in Eqs. (10), (11), and (12).

$$A_0 = \frac{w_{H_2O} \cdot m}{M_{H_2O}} \frac{RT}{V_g} \tag{10}$$

$$k_1 = G \cdot \frac{Q}{m} \cdot w_{e_{H_2O}} \cdot M_{H_2O} \tag{11}$$

$$k_2 = 7.5 \times 10^{-11} \left(\frac{mol}{s \cdot kPa} \right) \frac{RT}{V_g} \tag{12}$$

In these equations, G is the G-value for hydrogen production. The G-values are assigned in the database as 200 nmol W^{-1} s^{-1} for materials with chlorine or 5 nmol W^{-1} s^{-1} for materials without chlorine. The parameter $w_{e_{H_2O}}$ is the fraction of electrons associated with water, which is calculated using the number of electrons $\#e_i$ associated with each component i using Eq. (13).

$$w_{e_{H_2O}} = \frac{\dfrac{\#e_{H_2O}}{M_{H_2O}}}{\dfrac{w_{PuO_2} \cdot \#e_{PuO_2}}{M_{PuO_2}} + \dfrac{w_{U_3O_8} \cdot \#e_{U_3O_8}}{M_{U_3O_8}} + \dfrac{w_{NpO_2} \cdot \#e_{NpO_2}}{M_{NpO_2}} + \dfrac{w_{AmO_2} \cdot \#e_{AmO_2}}{M_{AmO_2}} + w_{salt}\dfrac{1}{2} + \dfrac{w_{H_2O} \cdot \#e_{H_2O}}{M_{H_2O}}} \tag{13}$$

The maximum hydrogen pressure $P_{H2,max}$ is calculated by substituting the parameters A_0, k_1, and k_2 into Eq. (14).

$$P_{H_2,max}(t) = \frac{A_0 k_1}{k_2 - k_1}\left[\left(\frac{k_1}{k_2}\right)^{\frac{k_1}{k_2 - k_1}} - \left(\frac{k_1}{k_2}\right)^{\frac{k_2}{k_2 - k_1}} \right] \tag{14}$$

The maximum container pressure $P_{IC,max}$ is calculated by summing the maximum hydrogen pressure $P_{H2,max}$, the container fill gas P_F, and the pressure of the other gases P_{other}, which was set to a constant of 50 kPa. The time to reach the maximum pressure is calculated by substituting the parameters k_1 and k_2 into Eq.(15).

$$t_{max} = \frac{\ln(k_2) - \ln(k_1)}{k_2 - k_1} \tag{15}$$